APPLICATION OF BAYESIAN FILTERS TO A ONE-DIMENSIONAL SOLIDIFICATION PROBLEM

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Abstract. *In this paper we applied two Bayesian filters to a solidification problem with the objective of estimate the location of the solidification front, as well as the intensity of a line heat sink. The main objective of this paper is to discuss and compare the performance of such two filters, namely: the SIR Filter (Sampling Importance Re-sampling Filter) and the ASIR (Auxiliary Sampling Importance Re-sampling) Filter.*

Keywords*: Bayesian inference, Sequential Monte Carlo, Importance sampling, Inverse Problems.*

1. INTRODUCTION

Sequential Monte Carlo (SMC) or Particle Filter Methods, which have been originally introduced in the beginning of the 50's, became very popular in the last few years in the statistical and engineering communities. Such methods have been widely used to deal with sequential Bayesian inference problems in fields like economics, signal processing, and robotics, among others. SMC Methods are an approximation of sequences of probability distributions of interest, using a large set of random samples, named particles. These particles are propagated along time with a simple Sampling Importance distribution, SI [1], and re-sampling techniques as well.

Hammersley and Hanscomb [2] presented a technique that used recursive Bayesian filters, together with Monte Carlo simulations, known as Sequential Importance Sampling (SIS). In such approach, the key idea was to represent the posterior probability function as a set of random samples associated with some weights, in order to calculate the estimates based on such samples and weights. Gordon et al. [3] added an extra step, named re-sampling, into the Sequential Importance Sampling method, to avoid the problem known as degeneration of particles. Such filter is known as Sampling Importance Re-sampling (SIR) Filter. In 2008, Orlande et al. [4] applied the SIR Filter to linear and non-linear heat conduction problems. In 2009, Vianna et al. [5] applied the Kalman and particle filters to a heat transfer problem, where the authors estimated the temperature field in a pipeline. The authors compared the results obtained through both methodologies. Later in 2010, Vianna et al [6] applied the particulate filter to a Pipe-in-Pipe system used in deepwater oil extraction, during a production shutdown. In 2010, Silva et al [7] compared different particle filter algorithms, as applied to an inverse one-dimensional, transient, heat conduction problem.

In this paper we apply the Sampling Importance Re-sampling (SIR) Filter and the Auxiliary Sampling Importance Re-sampling (ASIR) Filter to a non-linear solidification problem, in order to estimate a transient line heat sink as well as the solidification front in a phase change process. Simulated temperature measurements were used in the inverse analysis. The methods are compared in terms of computational time and accuracy of the recovered unknown.

2 PHYSICAL PROBLEM AND MATHEMATICAL FORMULATION

The physical problem analyzed in this paper consists of a one-dimensional transient heat solidification problem in a semi-infinite medium in cylindrical coordinates, as shown by Fig. 1. Initially, the entire medium is at a uniform temperature in the liquid phase and, at the initial time a heat sink is applied at $r=0$. The material then starts to solidify at $r=0$ and a solidification front moves away from the origin. The physical properties of liquid and solid phases are assumed constant. The material undergoing solidification is assumed to be a pure substance, so that phase change occurs at the temperature T_m.

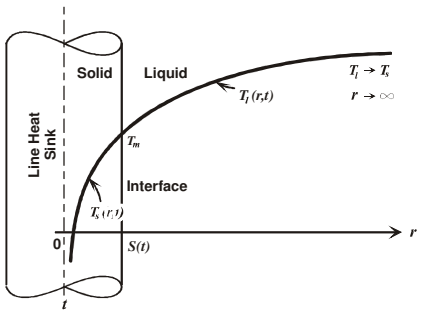


Figure 1. Solidification Problem [8]

The mathematical formulation for the solid phase is given as

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T_s(r,t)}{\partial r}\right)=\frac{1}{\alpha_s}\frac{\partial T_s(r,t)}{\partial t} \quad in \quad 0<r<S(t) \quad and \quad t>0 \tag{1.a}$$

while the liquid phase is described as

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T_l(r,t)}{\partial r}\right)=\frac{1}{\alpha_l}\frac{\partial T_l(r,t)}{\partial t} \quad in \quad S(t)<r<\infty \quad and \quad t>0 \tag{1.b}$$

$$T_l(r,t)\to T_i \quad in \quad r\to\infty \quad and \quad t>0 \tag{1.c}$$

$$T_l(r,t)=T_i \quad in \quad t=0 \quad and \quad r>0 \tag{1.d}$$

At the interface between liquid and solid phases, the following conditions must be satisfied

$$T_s(r,t)=T_l(r,t)=T_m \quad in \quad r=S(t) \quad and \quad t>0 \tag{1.e}$$

$$k_s\frac{\partial T_s(r,t)}{\partial r}-k_l\frac{\partial T_l(r,t)}{\partial r}=\rho L\frac{\partial S(t)}{\partial t} \quad in \quad r=S(t) \quad and \quad t>0 \tag{1.f}$$

An analytical solution of this problem can be obtained for this physical problem and it is given by [8]:

$$T_s(r,t)=T_m+\frac{Q_s}{4\pi k_s}\left[E_i\left(\frac{-r^2}{4\alpha_s t}\right)-E_i\left(-\lambda^2\right)\right] \quad 0<r<S(t) \tag{2.a}$$

$$T_l(r,t)=T_i-\frac{(T_i-T_m)}{E_i\left(\frac{-\lambda^2\alpha_s}{\alpha_l}\right)}\left[E_i\left(\frac{-r^2}{4\alpha_s t}\right)\right] \quad S(t)<r<\infty \tag{2.b}$$

where the eigenvalues λ and the solidification front S (t) are given by

$$\frac{Q}{4\pi k_s}e^{-\lambda^2}+\frac{k_l(T_i-T_m)}{E_i\left(\frac{-\lambda^2\alpha_s}{\alpha_l}\right)}e^{\frac{-\lambda^2\alpha_s}{\alpha_l}}=-\lambda^2\alpha_s\rho L \tag{3.a}$$

$$S(t)=2\lambda\sqrt{\alpha_s t} \tag{3.b}$$

In the above equations T_i is the uniform initial temperature, T_m is the melting temperature of the material, L is the latent heat of solidification of the material, ρ is the density, k_s and k_l are the thermal conductivities of the solid and

liquid phases, respectively, α_s and α_l are the thermal diffusivities of the solid and liquid phases, respectively, and T_s and T_l are temperatures of the solid and liquid phases, respectively.

3. STATE ESTIMATION

State estimation problems, also designated as nonstationary inverse problems [9], are of great interest in innumerable practical applications. In such kinds of problems, the available measured data is used together with prior knowledge about the physical phenomena and the measuring devices, in order to sequentially produce estimates of the desired dynamic variables. This is accomplished in such a manner that the error is minimized statistically [10].

Consider a model for the evolution of the state variables **x** in the form

$$\mathbf{x}_k = \mathbf{f}_k\left(\mathbf{x}_{k-1}, \mathbf{v}_k\right) \tag{4}$$

where **f** is, in the general case, a non-linear function of **x** and of the state noise or uncertainty vector given by $\boldsymbol{v}_k \in \mathbf{R}^{\mathbf{n}}$. The vector $\mathbf{x}_k \in \mathbf{R}^{\mathbf{n}}$ is called the state vector and contains the variables to be dynamically estimated. This vector advances in time in accordance with the *state evolution model* (4). The subscript k =1, 2, 3, …, denotes a time instant t_k in a dynamic problem.

The observation model describes the dependence between the state variable **x** to be estimated and the measurements z through the general, possibly non-linear, function $\boldsymbol{h}$. This can be represented by

$$\mathbf{z}_k = \mathbf{h}_k\left(\mathbf{x}_k, \mathbf{n}_k\right) \tag{5}$$

where $z_k \in \mathbf{R}^{\mathbf{n}_z}$ are available at times t_k, k=1, 2, 3,…. Eq. (5) is referred to as the *observation/measurement model*. The vector $\boldsymbol{n}_k \in \mathbf{R}^{\mathbf{n}_z}$ represents the measurement noise or uncertainty.

As per equations (4) and (5), the evolution and observation models are based on the following assumptions [9, 18-23, 28].

(a) The sequence $\mathbf{x}_k$ for k=1, 2, 3, …, is a Markovian process, that is,

$$\pi\left(\mathbf{x}_k \left| \mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_{k-1}\right.\right) = \pi\left(\mathbf{x}_k \left| \mathbf{x}_{k-1}\right.\right) \tag{6.a}$$

(b) The sequence $\mathbf{z}_k$ for k=1, 2, 3, …, is a Markovian process with respect to the history of $\mathbf{x}_k$, that is,

$$\pi\left(\mathbf{z}_k \left| \mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_k\right.\right) = \pi\left(\mathbf{z}_k \left| \mathbf{x}_k\right.\right) \tag{6.b}$$

(c) The sequence $\mathbf{x}_k$ depends on the past observations only through its own history, that is,

$$\pi\left(\mathbf{x}_k \left| \mathbf{x}_{k-1}, \mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_{k-1}\right.\right) = \pi\left(\mathbf{x}_k \left| \mathbf{x}_{k-1}\right.\right) \tag{6.c}$$

where $\pi(\mathbf{a}|\mathbf{b})$ denotes the conditional probability of **a** when **b** is given.

For the state and observation noises, the following assumptions are made [9, 18-23, 28]

(a) For $i \neq j$, the noise vectors $\mathbf{v}_i$ and $\mathbf{v}_j$, as well as $\mathbf{n}_i$ and $\mathbf{n}_i$, are mutually independent and also mutually independent of the initial state $\mathbf{x}_0$.

(b) The noise vectors $\mathbf{v}_i$ and $\mathbf{n}_j$ are mutually independent for all i and j.

Different problems can be considered for the evolution-observation models described above, such as [9, 18-23, 28]:

(i) The *prediction problem*, when the objective is to obtain $\pi(\mathbf{x}_k|\mathbf{z}_{1:k-1})$;

(ii) The *filtering problem*, when the objective is to obtain $\pi(\mathbf{x}_k|\mathbf{z}_{1:k})$;

(iii) The *fixed-lag smoothing problem*, when the objective is to obtain $\pi(\mathbf{x}_k|\mathbf{z}_{1:k+p})$, where $p \geq 1$ is the fixed lag.

(iv) The *whole-domain smoothing problem*, when the objective is to obtain $\pi(\mathbf{x}_k|\mathbf{z}_{1:K})$, where $\mathbf{z}_{1:K}=\{\mathbf{z}_i, i=1,...,K\}$ is the complete set of measurements.

We consider here the filtering problem. By assuming that $\pi(\mathbf{x}_0|\mathbf{z}_0) = \pi(\mathbf{x}_0)$ is available, the posterior probability density $\pi(\mathbf{x}_k|\mathbf{z}_{1:k})$ is then obtained with Bayesian filters in two steps [9, 18-23, 28]: *prediction and update*, as illustrated in figure 2.

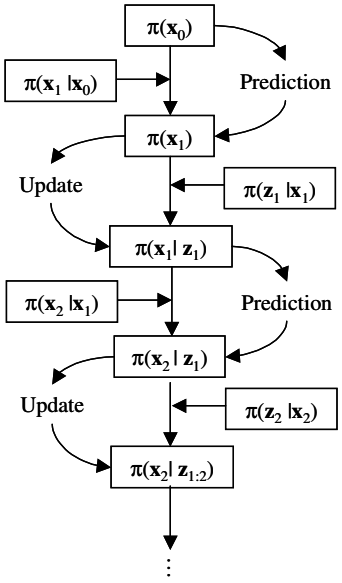


Figure 2. Prediction and update steps [28]

The most widely known Bayesian filter method is the Kalman filter [9, 18-22, 28-31]. However, the application of the Kalman filter is limited to linear models with additive Gaussian noises. Extensions of the Kalman filter were developed in the past for less restrictive cases by using linearization techniques. Similarly, Monte Carlo methods have been developed in order to represent the posterior density in terms of random samples and associated weights. Such Monte Carlo methods, usually denoted as particle filters among other designations found in the literature, do not require the restrictive hypotheses of the Kalman filter. Hence, particle filters can be applied to non-linear models with non-Gaussian errors [9, 18-22, 28-31].

The main idea in the particle filter is to represent the required posterior density function by a set of random samples with associated weights and to compute the estimates based on these samples and weights [9, 22-27,30,31]. Let $\{\mathbf{x}^i_k, i=0,...,N\}$ be the particles with associated weights $\{\mathbf{w}^i_k, i=0,...,N\}$ and $\mathbf{x}_{0:k}=\{\mathbf{x}_j, j=0,...,k\}$ be the set of all states up to t_k, where N is the number of particles. The weights are normalized, so that $\Sigma_i w^i_k=1$. Then, the posterior density at t_k can be discretely approximated by:

$$\pi\left(x_{0:k}\left|z_{1:k-1}\right.\right) \approx \sum_{i=1}^{I} w_k^i \delta\left(x_{0:k} - x_{0k}^i\right) \tag{7}$$

where $\delta(.)$ is the Dirac delta function. By taking hypotheses (6.a-c) into account, the posterior density in Eq. (7) can be written as $\pi(\mathbf{x}_k|\mathbf{z}_{1:k-1}) \approx \Sigma_i w^i_k \, \delta(\mathbf{x}_k - \mathbf{x}^i_k)$.

A common problem with the Particle Filter method is the degeneracy phenomenon, where after a few states all but one particle may have negligible weight. The degeneracy implies that a large computational effort is devoted to updating particles whose contribution to the approximation of the posterior density function is almost zero. This problem can be overcome by increasing the number of particles, or more efficiently by appropriately selecting the importance density as the prior density $\pi(\mathbf{x}_k|\mathbf{x}^i_{k-1})$. In addition, the use of the resampling technique is recommended to avoid the degeneracy of the particles [9, 22-27, 30, 31].

Resampling generally involves a mapping of the random measure $\{\mathbf{x}^i_k, w^i_k\}$into a random measure $\{\mathbf{x}^{i*}_k, N^{-1}\}$with uniform weights. It can be performed if the number of effective particles with large weights falls below a certain threshold number. Alternatively, resampling can also be applied indistinctively at every instant t_k, as in the *Sampling Importance Resampling* (SIR) algorithm [22, 23]. This algorithm can be summarized in the steps presented in Table 1, as applied to the system evolution from t_{k-1} to t_k.

Table 1 – SIR Algorithm [23].

Step 1
For i=1,...,N draw new particles $\mathbf{x}_k^i$ from the prior density $\pi(\mathbf{x}_k\|\mathbf{x}^i_{k-1})$ and then calculate some characterization of $\mathbf{x}_k$, given $\mathbf{x}^i_{k-1}$.
Step 2
For j=1,...,N draw particles $\mathbf{x}_k^i$ use the likelihood density to calculate the correspondent weights $w^j_k=\pi(\mathbf{z}_k\|\mathbf{x}^j_k)$ Calculate the total weight $t=\Sigma_i\, w^i_k$ and then normalize the particle weights, that is, for i=1,...,N let $w^i_k = t^{-1}\, w^i_k$
Step 3
Resample the particles as follows :
Construct the cumulative sum of weights (CSW) by computing $c_i=c_{i-1}+w^i_k$ for i=1,...,N, with c_0=0
Let i=1and draw a starting point u_1 from the uniform distribution U[0,N^{-1}]
For j=1,...,N
Move along the CSW by making $u_j=u_1+N^{-1}(j-1)$
While $u_j>c_i$ make $i=i+1$ Assign sample $x^j_k=x^i_k$ Assign sample $w^j_k=N^{-1}$
Step 4
Calculate the total weight $t=\Sigma_j\, w^j_k$ and then normalize the particle weights, that is, for j=1,...,N let $w^j_k = t^{-1}\, w^j_k$

Although the resampling step reduces the effects of the degeneracy problem, it may lead to a loss of diversity and the resultant sample can contain many repeated particles. This problem, known as sample impoverishment, can be severe in the case of small evolution model noise. In this case, all particles collapse to a single particle within few instants t_k. Another drawback of the particle filter is related to the large computational cost due to the Monte Carlo method, which may limit its application only to fast computing problems.

Different algorithms for the implementation of the particle filter can be found in [31], including those that permit the simultaneous estimation of constant parameters appearing in the model and the transient states. One of such algorithms is the Auxiliary *Sampling Importance Resampling* (ASIR) Method, which is summarized in table 2.

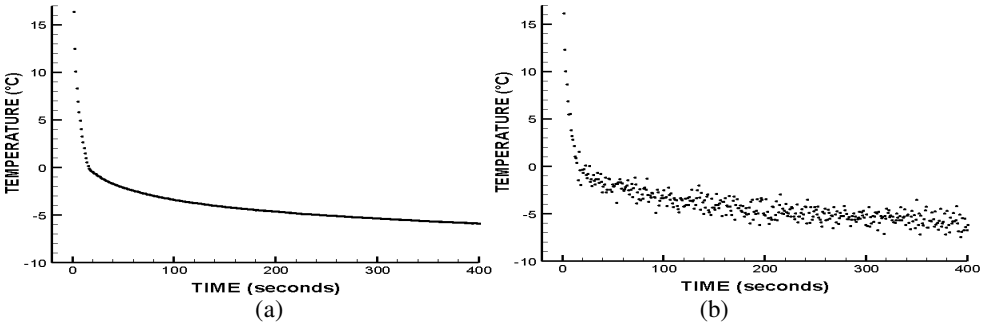
Table 2 – ASIR Algorithm [22, 23]

Step 1
For i=1,...,N draw new particles $\mathbf{x}_k^i$ from the prior density $\pi(\mathbf{x}_k\|\mathbf{x}^i_{k-1})$ and then calculate some characterization of $\mathbf{x}_k$, given $\mathbf{x}^i_{k-1}$, as for example the mean μ^i_k=E[$\mathbf{x}_k\|\mathbf{x}^i_{k-1}$]. Then use the likelihood density to calculate the correspondent weights $w^i_k=\pi(\mathbf{z}_k\|\mu^i_k)w^i_{k-1}$
Step 2
Calculate the total weight $t=\Sigma_i\, w^i_k$ and then normalize the particle weights, that is, for i=1,...,N let $w^i_k = t^{-1}\, w^i_k$
Step 3
Resample the particles as follows :
Construct the cumulative sum of weights (CSW) by computing $c_i=c_{i-1}+w^i_k$ for i=1,...,N, with c_0=0
Let i=1and draw a starting point u_1 from the uniform distribution U[0,N^{-1}]
For j=1,...,N
Move along the CSW by making $u_j=u_1+N^{-1}(j-1)$
While $u_j>c_i$ make $i=i+1$ Assign sample $x^j_k=x^i_k$ Assign sample $w^j_k=N^{-1}$ Assign parent $i^{(j)}=i$
Step 4
For j=1,...,N draw particles x_k^j from the prior density $\pi\left(\mathrm{x_k}\,\middle|\,x_{k-1}^{i(j)}\right)$, using the parent $i^{(j)}$, and then use the likelihood density to calculate the correspondent weights $w_k^j = \dfrac{\pi\left(\mathrm{z_k}\,\middle|\,x_k^j\right)}{\pi\left(\mathrm{z_k}\,\middle|\,\mu_{k-1}^{i(j)}\right)}$
Step 5
Calculate the total weight $t=\Sigma_j\, w^j_k$ and then normalize the particle weights, that is, for j=1,...,N let $w^j_k = t^{-1}\, w^j_k$

In ASIR filter algorithm, the index $i^{(j)}$ are obtained by resampling (i.e. after resampling the particles with higher weights and their index are obtained. These index are $i^{(j)}$, j = 1, .. N). According to [22], the advantage of the ASIR algorithm over the *Sampling Importance Resampling* (SIR) algorithm is that it naturally generates points from the sample at k-1, which, conditioned on the current measurement, are most likely to be close to the true state. Still, as described in [22], ASIR can be viewed as resampling at the previous time step, based on some point estimates μ^i_k that characterize $\pi(\mathbf{x}_k\|\mathbf{x}^i_{k-1})$. The use of ASIR is limited to small process noise. For a large process noise, a single point μ^i_k is not able to characterize $\pi(\mathbf{x}_k\|\mathbf{x}^i_{k-1})$.

4. RESULTS AND DISCUSSIONS

The physical problem defined by Eqs. (1.a-f) was solved analytically, where we used the following data, corresponding to solidifying water: $T_i = 25°C$, $T_m = 0°C$, $\alpha_s = 0.00118\frac{m^2}{s}$, $\alpha_l = 0.000146\frac{m^2}{s}$, $k_s = 2.22\frac{w}{m°c}$, $k_l = 0.61\frac{w}{m°c}$, $\rho = 997.1\frac{kg}{m^3}$, $L = 80\ \frac{\mathrm{J}}{\mathrm{kg}}$. The line heat sink was supposed to have a constant value equals to $\mathrm{Q} = 50\frac{\mathrm{W}}{\mathrm{m}}$. In this work, the measurements (for the observation model) were obtained at r=0.01 m. The simulated noisy measurements were uncorrelated, additive, Gaussian, with zero mean and constant standard deviation equal to 5% of the maximum temperature. Figures 3.a,b show the transient measurements obtained after applying such constant line heat sink, with and without errors, respectively.



(a) (b)

Figure 3: Simulated temperature measurements (a) errorless and (b) Gaussian with standard deviation of 5% of the maximum temperature

A random walk model was used for the evolution model involving the estimation of an unknown line heat sink, as given by Eq. (8.a). In this equation, σ is the standard deviation used to advance the line heat sink in time, taken to be equal to 0.25 W/m, while W are random numbers with normal distribution, zero mean, and unitary standard deviation. Equation (8.b) shows the evolution model for the solidification front, obtained by re-writing equation (3.b) in an appropriate form for the application of the particle filter algorithms presented above. Uncertainties in the evolution model for the solidification front were taken into account. The α_s is standard deviation for $S(t)$, used to advance the solidification front, was taken as 1% of the maximum value of the solidification front.

$$Q(t_k) = Q(t_{k-1}) + \sigma W \tag{8.a}$$

$$S(t_k) = S(t_{k-1}) + 2\lambda\sqrt{\alpha_s}\left(\sqrt{t_k} - \sqrt{t_{k-1}}\right) + \sigma_s W \tag{8.b}$$

To better analyze the results generated we calculate the root mean square error between the simulated and observed values, as given by equation (8.c)

$$RMS = \sqrt{\frac{1}{M}\sum_{j=1}^{M}\left(X_m(j) - X_0(j)\right)^2} \tag{8.c}$$

where X_m represent the simulated values, X_0 represent the observed values and M is the total points.

The two filters previously presented were applied to the problem of estimating the transient line heat sink as well as the solidification front. Table 3 summarizes the cases examined, as well as their results for CPU time and RMS errors. Table 3 shows that the SIR filter presented a computational time varying from 0.008 to 11.047 minutes, when the number of particles varied from 100 to 5000. Also, the variation of the RMS for the estimation of the solidification front varied from $9x10^{-3}$ m to $1x10^{-4}$ m. On the other hand, by applying the ASIR filter with only 100 particles, the computational time was of 0.161 minutes, with an RMS error of $2x10^{-5}$ m to estimate the solidification front. In this same table, one can notice that the RMS error for recovering the line heat sink also was much smaller for the ASIR filter than for SIR filter. Thus, the ASIR filter was more efficient in recovering the unknown quantities, with a much smaller number of particles than those required for the SIR filter.

Table 3. Computational time and RMS errors

Bayesian filter	**Number of Particles (NP)**	**Time**	**RMS error for the solidification front (m)**	**RMS error for the line heat sink intensity (W/m)**
SIR	100	0.008 min.	$9x10^{-3}$	1.55
SIR	1000	0.997 min.	$2x10^{-3}$	1.78
SIR	5000	11.047 min.	$1x10^{-4}$	0.34
ASIR	100	0.161 min.	$7.9x10^{-5}$	0.15

Figures 4 and 5 show the estimated and real values for the transient variations of the solidification front and the line heat sink, respectively. It can be seen that the ASIR filter outperforms the SIR filter, even when a large number of particles is used in the later one. In these figure, the mean values are represented by the symbols, while de real values are represented by a continuous line. Error bars are also included, for a 99% confidence interval. Whereas the estimated location of the solidification front is reasonably well captured for all filters, the value of the line heat sink is completed overestimated by the SIR filter with 100 or 1000 particles. Only when the number of particles is increased to 5000, the real value of the line heat sink is located within the error bars of the estimated value. The ASIR filter, on the other hand, is able to capture the mean value of the line heat sink superbly well, even for a number of particles as small as 100.

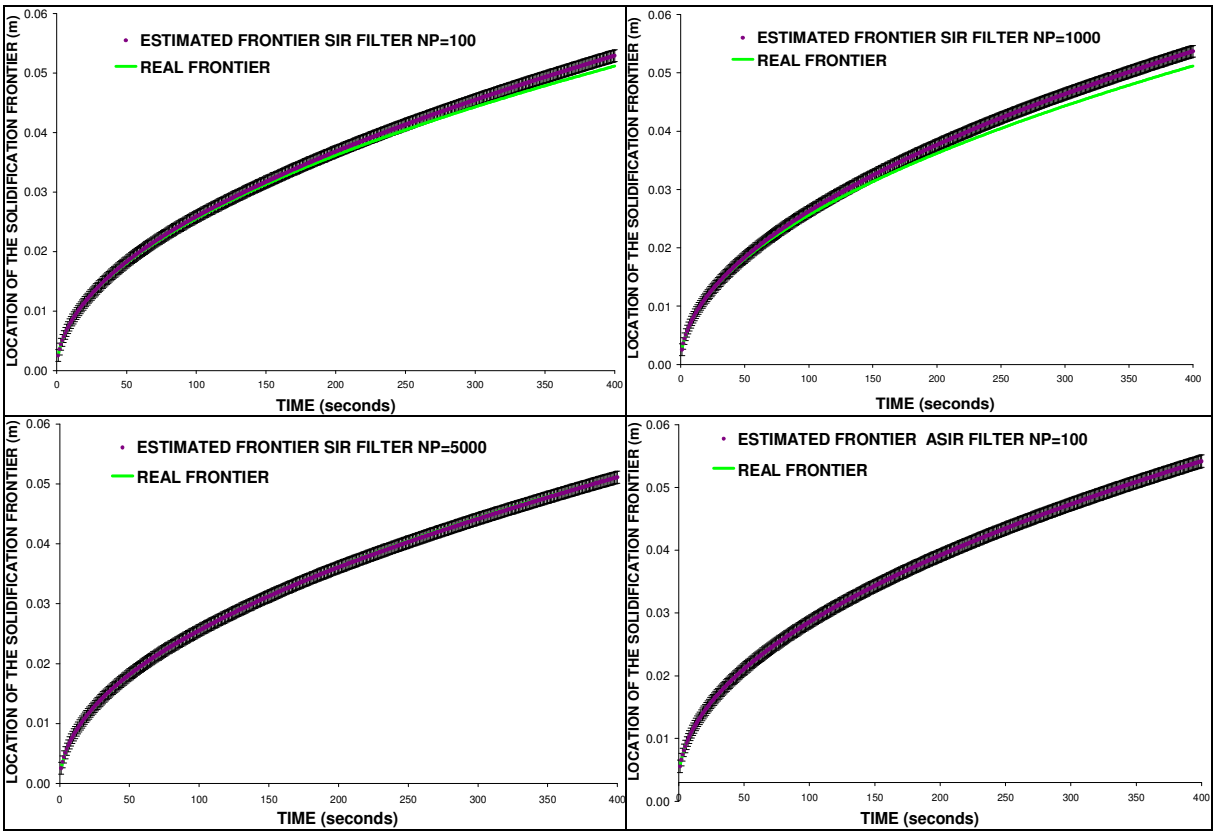


Figure 4. Location of the solidification front

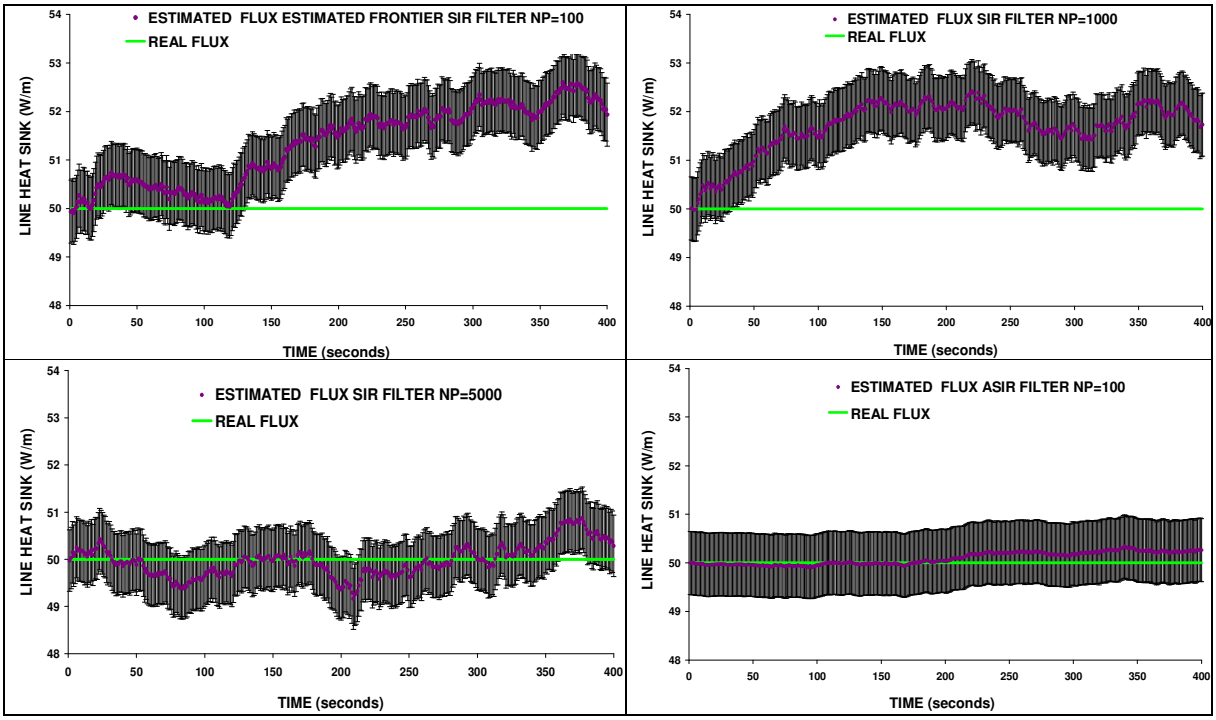


Figure 5. Line Heat Sink Intensity

5. CONCLUSIONS

In this paper we applied two Bayesian particle filters algorithms - the SIR and ASIR filters - to a one dimensional heat transfer problem with solidification. It was shown that the ASIR algorithm was substantially superior to the SIR algorithm, being capable of recovering both the solidification front and an unknown line heat sink, with a number of particles 50 times smaller than for the SIR filter. Also, the computational time involved in the use of the ASIR filter was much smaller than the SIR filter, for the same order of accuracy of the results.

6. ACKNOWLEDGEMENTS

The authors would like to thank the Brazilian agencies for the fostering of science, *Conselho Nacional de Desenvolvimento Científico e Tecnológico* (CNPq), *Coordenação de Aperfeiçoamento de Pessoal de Nível Superior* (CAPES) and *Fundação Carlos Chagas Filho de Amparo à Pesquisa do Estado do Rio de Janeiro* (FAPERJ), for the financial support for this work.

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